Available online at www.elixirpublishers.com (Elixir International Journal)

Computational Chemistry

Elixir Comp. Chem. 110 (2017) 48184-48185

ISSN: 2229-712X

Computational Chemistry

Matthew N. O. Sadiku[1], Sarhan M. Musa[1] and Osama M. Musa[2]
[1]Roy G. Perry College of Engineering, Prairie View A&M University Prairie View, TX 77446.
[2]Ashland Inc. Bridgewater, NJ 08807.

ARTICLE INFO

Article history:
Received: 1 August 2017;
Received in revised form:
30 August 2017;
Accepted: 8 September 2017;

Keywords
Computational Chemistry,
Computational Science,
Scientific Computing,
Molecular Modeling.

ABSTRACT

Computational chemistry is rapidly emerging as a new branch of chemistry. It is basically the application of chemical, mathematical, and information technology principles to the solution of complex chemical problems. It uses computers to the 3-dimensional structures and key properties of molecules and materials. This information can provide critical insight and better mechanistic understanding of complex chemical systems, leading to discovery and development new materials with superior properties. Computational chemistry is widely used in many multidisciplinary fields with applications in chemistry, biology, and material science. This paper provides a brief introduction to computational chemistry.

Introduction

Many disciplines have undergone a computational turn in the past decades. The recent computational turn has produced subdisciplines such as computational humanities, computational sociology, computational economics, computational mechanics, computational fluid dynamics, computational science, computational electromagnetics, computational medicine, human computation, and computational chemistry. Computational chemistry (CC) is part the general area of computational science. It refers to using computers to model, simulate, and solve chemical problems. It can also be described as computation methods aimed at understanding molecules and materials. Computational chemists may use supercomputers to solve problems. Computational results normally complement the information obtained from theoretical chemistry and chemical experiments.

The term "theoretical chemistry" may be regarded as a mathematical description of chemistry, whereas "computational chemistry" can be described as developing mathematical method to the extent that the result can be automated for implementation on a computer [1]. Computational chemistry is not being confused with computer science, although professionals in the two fields often collaborate. We must keep in mind that computers do not solve problems, humans do and computers just generate data.

Although chemists have been doing computations for ages, the field we refer to today as "computational chemistry" is a product of the digital age. With the development of digital computers in the 1940s, the solutions of complex chemical systems began to be realizable. In the early 1950s, chemists began to use digital computers extensively. A brief history of early developments in CC is given in [2]. The chemical community has taken advantage of all advances in software and hardware in promoting the use of computational chemistry in all aspects of chemical research.

Computational chemistry has become a vital collaborator with experimental chemistry, whether it be physical chemistry, organic chemistry, biochemistry, medicinal chemistry or analytical chemistry. It has attracted several Nobel Prize awards. Over the years, Royal Swedish Academy of Science has awarded several Nobel Prizes in chemistry making groundbreaking contributions to computational chemistry. For example, three computational chemists, Paul Crutzen, Mario Molina, and F. Sherwood Rowland, won the Chemistry Nobel in 1995 for their work of depletion of the ozone layer. Their work led to the ban on chlorofluorocarbons (CFCs) which saved thousands of lives by reducing the risk of skin cancer. More recently, the 2013 Noble prize in Chemistry was awarded to Martin Karplus, Michael Levitt and Arieh Warshel for their work on developing computational methods to study complex chemical systems.

Computation Tools

Computational tools used by chemists include electronic structure methods, molecular dynamics simulations, cheminformatics (a field that combines laboratory data, chemical modeling, and information science methods), data analysis, visualization and full statistical analysis. The length and time scale of the chemical process of interest and the particular application will determine computational method used. For example, if the system being studied can be represented by a model that is less than 1 nanometer (nm), or the process being studied involves electrons, then quantum mechanical electronic structure methods are the best choice. If the system being studied is represented by models that are greater 100nm or involve chemical diffusion or phase behavior, then mesoscale dynamics are often employed. As shown in Figure 1, the modeling strategy may require a hierarchical scheme [3].

Several comprehensive computational chemistry software packages or programs exist today. These software packages include Gaussian, GaussSum, GAMESS, GRAMPS, MOPAC, Spartan, Sybyl, AMBER, and Aces4.

Tele:
E-mail address: omusa@ashland.com

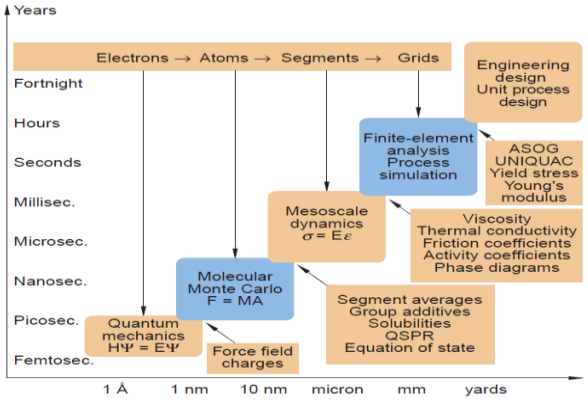

Figure 1. Hierarchy of materials simulation [3].

The programming languages used in developing these packages include FORTRAN, C, C++, and Python. Several commercial software manufacturers market a variety of computational chemistry computer programs that are increasingly being used in education. Computational chemists may freely choose from this wide variety of computational chemistry packages [4].

Applications

Computational chemistry is used in studying the fundamental properties of atoms and molecules using quantum mechanics and thermodynamics. Computational chemistry can also be applied to solid state physical problems. Computational chemistry is typically to:

- Visualize chemical structure and dynamics
- Study molecular conformations and flexibility
- Determine electronic properties such as chemical reactivity, polarity and spectroscopy
- Determine dynamic properties such as molecular diffusion and isomerization
- Characterize and quantify intermolecular interactions, molecular binding, adhesion, and surface chemistry
- Study phase morphology and transitions
- Design of new medicine
- Develop new catalysts
- Uncover hidden relationships between molecular structure, process, and properties.

It influences our understanding of the way the world works and helps manufacturers design more productive and efficient processes. It can help design new materials and improve manufacturing efficiency and material design. Combustion is another area where the computational approach really shines.

The application of computational chemistry in the area of carotenoids has gained attention in the last two decades. The use of computational chemistry in drug design has become a standard practice. However, computational chemistry's role in drug design is experiencing some fundamental changes [3].

Conclusion

Computational chemistry has come of age. It has become an essential tool for chemists. The rapid advances in hardware and software can propel computational chemistry to be a strategic tool for productivity for chemists. Calculations with efficient parallel implementation approaching the Petascale level are now being made. For example, researchers at D.E. Shaw Research have used very large scale molecular dynamics to study the structure and dynamics of proteins and how they function [8]. Such a computation would be impossible without massively parallel supercomputer technology. The impact of these advances will be broad and encompassing, because chemistry is so central to diverse areas such as biological systems, pharmaceutical industry, and chemical manufacturing [5].

Because computational chemistry is integral to modern chemistry research, chemistry education should reflect this. It is prudent and imperative that students in the modern undergraduate curriculum become used to performing basic calculations using computational software packages. They should use computational chemistry to obtain a deeper understanding of their experimental work throughout the entire curriculum [6]. The pharmaceutical industry is a major employer of computational chemists.

Computational knowledge from one researcher to another is transmitted through conferences and journal. The Journal of Computational Chemistry publishes research works on all aspects of numerical solution of chemical problems.

References

[1]"Computational chemistry" Wikipedia, the free encyclopedia https://en.wikipedia.org/wiki/Computational_chemistry

[2] H. S. Rzepa, "The Internet as a computational chemistry tool," Journal of Molecular Structure (Theochem), vol 398-399, 1997, pp. 27-33.

[3] S. Dasgupta, "The role and challenges of computational chemistry in industrial problems," Computing in Science and Engineering, November/December 2000, pp. 52-60.

[4] N. M. O'Boyle, A. L. Tenderholt, and K. M. Langner, "Software news and updates cclib: a library for package-independent computational chemistry algorithms," Journal of Computational Chemistry, vol. 29, no. 5, 2007, pp. 839-845,

[5]D.G. Truhlar and V. McKoy, "Computational Chemistry," Computing in Science and Engineering, November/December 2000, pp. 19-21.

[6] Z. L. Gasyna and S. A. Rice,"Computational chemistry in the undergraduate chemistry curriculum: development of a comprehensive source formula," Journal of Chemical Education, vol. 76, no. 7, July 1999, pp. 1023-1029.

[7] N. H. Martin, "Integration of computational chemistry into the chemistry curriculum," Journal of Chemical Education, vol. 75, no. 2, February 1998, pp. 241-243.

[8] Kresten Lindorff-Larsen, Paul Maragakis, Stefano Piana, and David E. Shaw, "Picosecond to Millisecond Structural Dynamics in Human Ubiquitin," The Journal of Physical Chemistry B, vol. 120, no. 33, 2016, pp. 8313–8320.

Authors

Matthew N.O. Sadiku is a professor in the Department of Electrical and Computer Engineering at Prairie View A&M University, Prairie View, Texas. He is the author of several books and papers. His areas of research interest include computational electromagnetics and computer networks. He is a fellow of IEEE.

Sarhan M. Musa is a professor in the Department of Engineering Technology at Prairie View A&M University, Texas. He has been the director of Prairie View Networking Academy, Texas, since 2004. He is an LTD Sprint and Boeing Welliver Fellow.

Osama M. Musa is currently Vice President and Chief Technology Officer for Ashland Inc. Dr. Musa also serves as a member of the Advisory Board at Manhattan College's Department of Electrical and Computer Engineering as well as a member of the Board of Trustees at Chemists' Club of NYC. Additionally, he sits on the Advisory Board of the International Journal of Humanitarian Technology (IJHT).